Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 69.3 °C

Global applicability domain: Inside

Local applicability domain index: 8.63e-01

Confidence level: 6.17e-01

Nearest Neighbors from the Training Set

Image not found	Image not found	Image not found
Methoxyphenone	1-Naphthalenecarboxaldehyde, 2-ethoxy-	4-Methoxybenzophenone
Measured: 62.3	**Measured:** 115	**Measured:** 61.5
Predicted: 67.5	**Predicted:** 69.9	**Predicted:** 55.8